

STN
current of species
hml 9/20/07

=> d his

(FILE 'HOME' ENTERED AT 21:58:13 ON 20 SEP 2007)

FILE 'REGISTRY' ENTERED AT 21:58:34 ON 20 SEP 2007

L1 STRUCTURE UPLOADED
L2 15 S L1
L3 274 S L1 SSS FULL
L4 STRUCTURE UPLOADED
L5 1 S L4
L6 3 S L4 SSS FULL
L7 0 S L3 SUB=L6 FULL
L8 STRUCTURE UPLOADED
L9 0 S L8
L10 2 S L8 SSS FULL
L11 0 S L3 SUB=L10 FULL
L12 0 S L10 SUB=L3 FULL

FILE 'HCAPLUS' ENTERED AT 22:02:54 ON 20 SEP 2007

L13 45 S L3

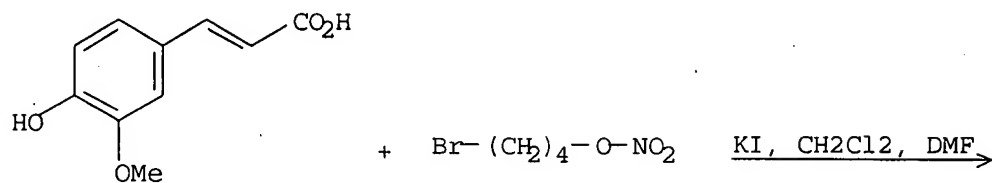
FILE 'STNGUIDE' ENTERED AT 22:04:42 ON 20 SEP 2007

FILE 'CASREACT' ENTERED AT 22:11:16 ON 20 SEP 2007

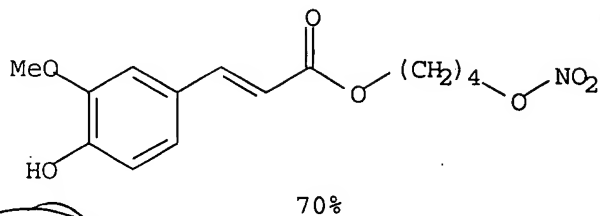
L14 STRUCTURE UPLOADED
L15 0 S L14
L16 2 S L14 SSS FULL
L17 STRUCTURE UPLOADED
L18 0 S L17
L19 2 S L17 SSS FULL
L20 STRUCTURE UPLOADED
L21 0 S L20
L22 6 S L20 SSS FULL

L16 ANSWER 1 OF 2 CASREACT COPYRIGHT 2007 ACS on STN

RX(3) OF 6



K



Int App

REF: PCT Int. Appl., 2006056535, 01 Jun 2006
CON: STAGE(1) room temperature -> 40 deg C; 136 hours, 40 deg C

=> fcrdref 1-2

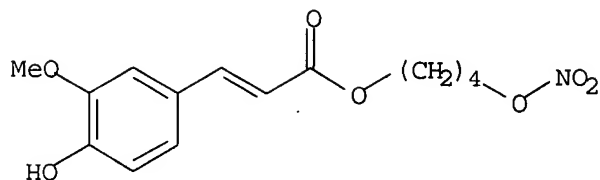
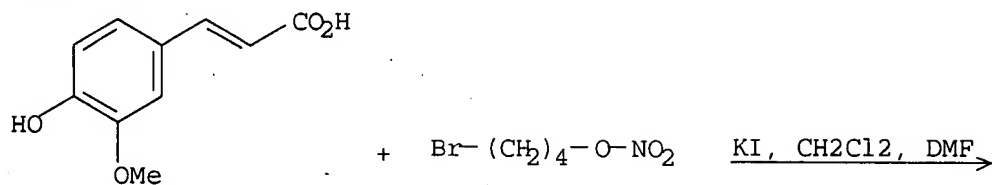
FCRDREF IS NOT A RECOGNIZED COMMAND

The previous command name entered was not recognized by the system.
For a list of commands available to you in the current file, enter
"HELP COMMANDS" at an arrow prompt (=>).

=> d 116 fcrdref 1-2

L16 ANSWER 1 OF 2 CASREACT COPYRIGHT 2007 ACS on STN

RX(3) OF 6



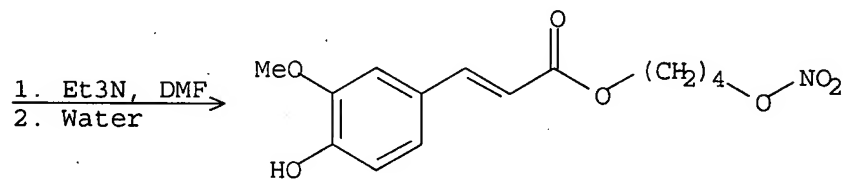
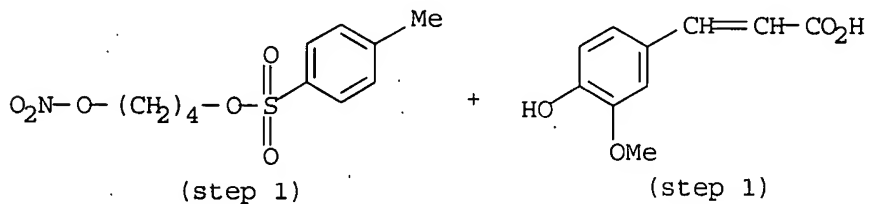
70%

REF: PCT Int. Appl., 2006056535, 01 Jun 2006

CON: STAGE(1) room temperature -> 40 deg C; 136 hours, 40 deg C

L16 ANSWER 2 OF 2 CASREACT COPYRIGHT 2007 ACS on STN

RX(1) OF 6



70%

REF: PCT Int. Appl., 2004020385, 11 Mar 2004

CON: STAGE(1) room temperature; 72 hours, room temperature;
room temperature; 24 hours, room temperature
STAGE(2) room temperature

=>

Uploading C:\Program Files\Stnexp\Queries\2007 cases\10522986\species but generic.str

10/522986 NITROOXYALKYL SUBTD ESTERS

L17 STRUCTURE UPLOADED

=> s 117

SAMPLE SEARCH INITIATED 22:14:18 FILE 'CASREACT'

SCREENING COMPLETE - 59 REACTIONS TO VERIFY FROM

2 DOCUMENTS

100.0% DONE 59 VERIFIED 0 HIT RXNS

0 DOCS

SEARCH TIME: 00.00.01

FULL FILE PROJECTIONS: ONLINE **COMPLETE**

BATCH **COMPLETE**

PROJECTED VERIFICATIONS: 720 TO 1640

PROJECTED ANSWERS: 0 TO 0

L18 0 SEA SSS SAM L17 (0 REACTIONS)

=>

=> s 117 sss full

FULL SEARCH INITIATED 22:14:31 FILE 'CASREACT'

SCREENING COMPLETE - 948 REACTIONS TO VERIFY FROM

58 DOCUMENTS

100.0% DONE 948 VERIFIED 6 HIT RXNS

2 DOCS

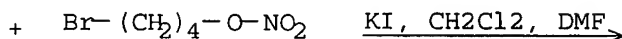
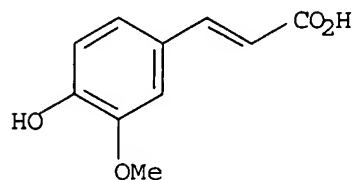
SEARCH TIME: 00.00.01

L19 2 SEA SSS FUL L17 (6 REACTIONS)

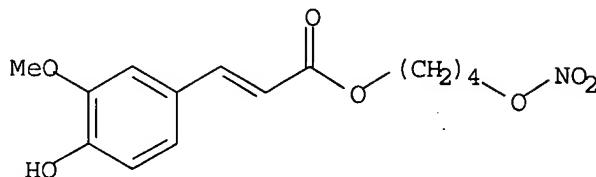
=> d 119 fcrdref 1-2

L19 ANSWER 1 OF 2 CASREACT COPYRIGHT 2007 ACS on STN

RX(3) OF 6



K



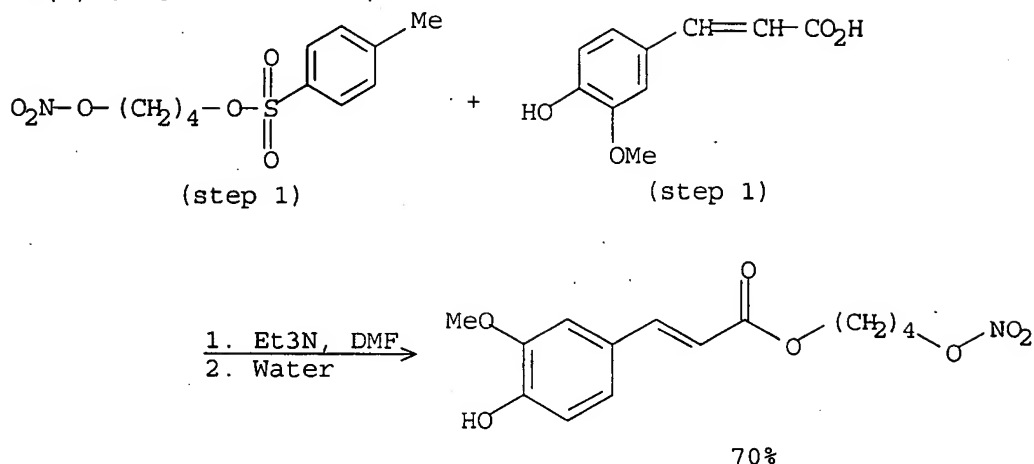
70%

REF: PCT Int. Appl., 2006056535, 01 Jun 2006

CON: STAGE(1) room temperature -> 40 deg C; 136 hours, 40 deg C

L19 ANSWER 2 OF 2 CASREACT COPYRIGHT 2007 ACS on STN

RX(1) OF 6



REF: PCT Int. Appl., 2004020385, 11 Mar 2004
 CON: STAGE(1) room temperature; 72 hours, room temperature;
 room temperature; 24 hours, room temperature
 STAGE(2) room temperature

=>

Uploading C:\Program Files\Stnexp\Queries\2007 cases\10522986\generic.str

L20 STRUCTURE UPLOADED

=> s l20

SAMPLE SEARCH INITIATED 22:15:30 FILE 'CASREACT'

SCREENING COMPLETE - 3482 REACTIONS TO VERIFY FROM 189 DOCUMENTS

100.0% DONE 3482 VERIFIED 0 HIT RXNS 0 DOCS
 SEARCH TIME: 00.00.01

FULL FILE PROJECTIONS: ONLINE **COMPLETE**
 BATCH **COMPLETE**

PROJECTED VERIFICATIONS: 66109 TO 73171

PROJECTED ANSWERS: 0 TO 0

L21 0 SEA SSS SAM L20 (0 REACTIONS)

=> s l20 sss full

FULL SEARCH INITIATED 22:15:39 FILE 'CASREACT'

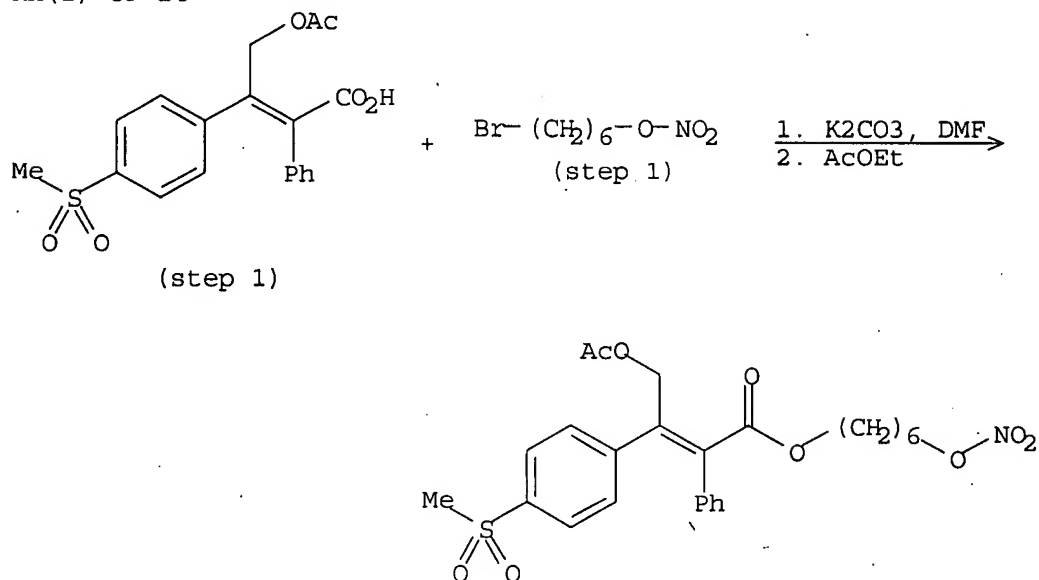
SCREENING COMPLETE - 63398 REACTIONS TO VERIFY FROM 3265 DOCUMENTS

100.0% DONE 63398 VERIFIED 122 HIT RXNS 6 DOCS
 SEARCH TIME: 00.00.03

L22 6 SEA SSS FUL L20 (122 REACTIONS)

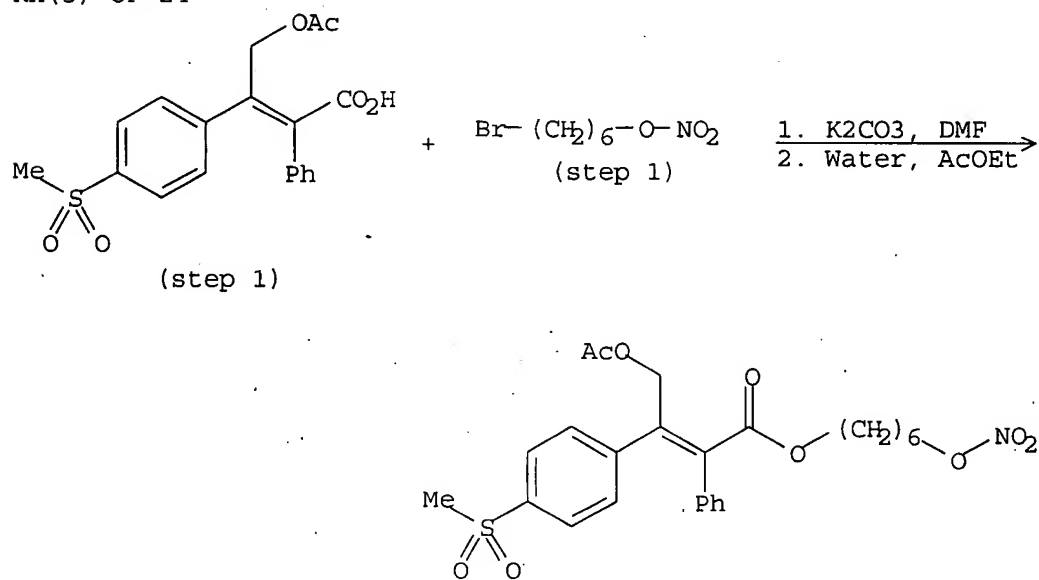
=> d l22 fcrdref 1-22

RX(1) OF 24



REF: Journal of Organic Chemistry, 71(2), 480-491; 2006
 CON: STAGE(1) room temperature; 2 - 3 hours, 20 - 22 deg C
 STAGE(2) 0.5 hours, <30 deg C

RX(5) OF 24



REF: U.S. Pat. Appl. Publ., 2005192346, 01 Sep 2005

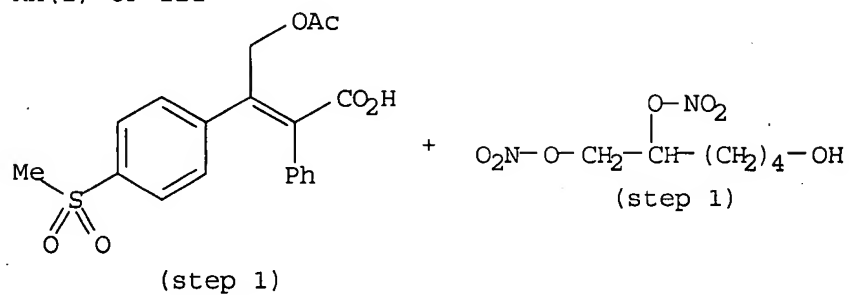
NOTE: work-up

CON: STAGE(1) 2 - 3 hours, 20 - 22 deg C

STAGE(2) 0.5 hours, <30 deg C

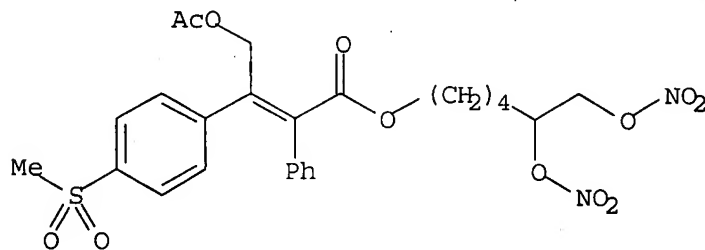
L22 ANSWER 3 OF 6 CASREACT COPYRIGHT 2007 ACS on STN

RX(1) OF 121



1. 4-DMAP, EDAP,
CH₂Cl₂
2. AcOH

RX(1) OF 121

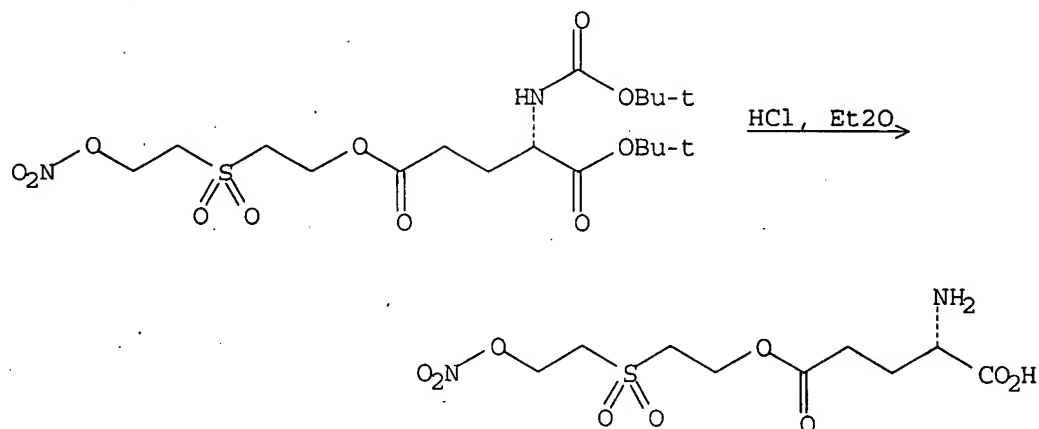


REF: PCT Int. Appl., 2005070874, 04 Aug 2005

CON: 3 hours, room temperature

L22 ANSWER 4 OF 6 CASREACT COPYRIGHT 2007 ACS on STN

RX(4) OF 233



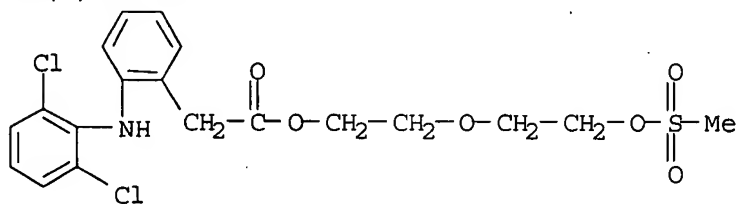
HCl

REF: PCT Int. Appl., 2005030135, 07 Apr 2005

CON: 40 hours, room temperature

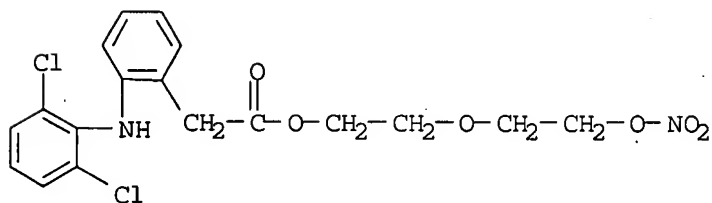
L22 ANSWER 5 OF 6 CASREACT COPYRIGHT 2007 ACS on STN

RX(2) OF 24



(step 1)

1. Bu4N.NO3, NaNO3,
S:123-86-4, MeCN
2. Water

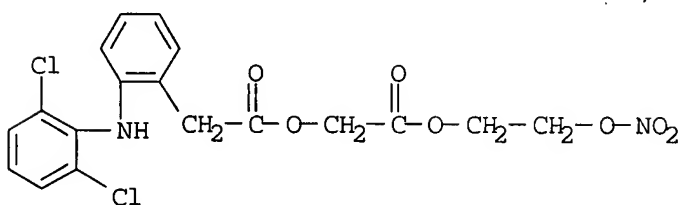
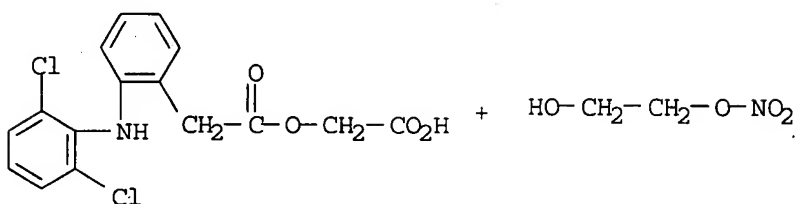


93%

REF: PCT Int. Appl., 2004026808, 01 Apr 2004

CON: STAGE(1) 60 deg C; 50 hours, 87 deg C

RX(1) OF 4



69%

REF: Eur. Pat. Appl., 738706, 23 Oct 1996

equiv to US 5844696

=> d his

(FILE 'HOME' ENTERED AT 21:58:13 ON 20 SEP 2007)

FILE 'REGISTRY' ENTERED AT 21:58:34 ON 20 SEP 2007

L1 STRUCTURE UPLOADED
 L2 15 S L1
 L3 274 S L1 SSS FULL
 L4 STRUCTURE UPLOADED
 L5 1 S L4
 L6 3 S L4 SSS FULL
 L7 0 S L3 SUB=L6 FULL
 L8 STRUCTURE UPLOADED
 L9 0 S L8
 L10 2 S L8 SSS FULL
 L11 0 S L3 SUB=L10 FULL
 L12 0 S L10 SUB=L3 FULL

FILE 'HCAPLUS' ENTERED AT 22:02:54 ON 20 SEP 2007

L13 45 S L3

FILE 'STNGUIDE' ENTERED AT 22:04:42 ON 20 SEP 2007

FILE 'CASREACT' ENTERED AT 22:11:16 ON 20 SEP 2007

L14 STRUCTURE UPLOADED
 L15 0 S L14
 L16 2 S L14 SSS FULL
 L17 STRUCTURE UPLOADED
 L18 0 S L17

10/522986 NITROOXYALKYL SUBTD ESTERS

L19	2 S L17 SSS FULL
L20	STRUCTURE UPLOADED
L21	0 S L20
L22	6 S L20 SSS FULL

=>

10/522986 NITROOXYALKYL SUBTD ESTERS

=>

Uploading C:\Program Files\Stnexp\Queries\2007 cases\10522986\electd species
Example2B.str

L14 STRUCTURE UPLOADED

=> s l14

SAMPLE SEARCH INITIATED 22:11:47 FILE 'CASREACT'

SCREENING COMPLETE - 0 REACTIONS TO VERIFY FROM 0 DOCUMENTS

100.0% DONE 0 VERIFIED 0 HIT RXNS 0 DOCS

SEARCH TIME: 00.00.01

FULL FILE PROJECTIONS: ONLINE **COMPLETE**

 BATCH **COMPLETE**

PROJECTED VERIFICATIONS: 0 TO 0

PROJECTED ANSWERS: 0 TO 0

L15 0 SEA SSS SAM L14 (0 REACTIONS)

=> s l14 sss full

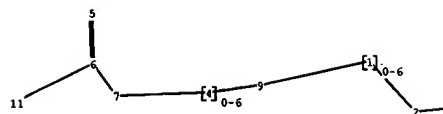
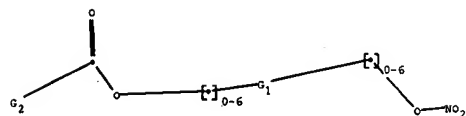
FULL SEARCH INITIATED 22:11:55 FILE 'CASREACT'

SCREENING COMPLETE - 55 REACTIONS TO VERIFY FROM 5 DOCUMENTS

100.0% DONE 55 VERIFIED 6 HIT RXNS 2 DOCS

SEARCH TIME: 00.00.01

L16 2 SEA SSS FUL L14 (6 REACTIONS)



chain nodes :

1 2 3 4 5 6 7 9 11

chain bonds :

1-2 1-9 2-3 4-9 4-7 5-6 6-7 6-11

exact/norm bonds :

1-2 1-9 2-3 4-9 4-7 5-6 6-7 6-11

G1:O,S,SO2,NH,Cb,Cy,Hy,Ak

G2:A,Cb,Cy,Hy,Ak

Match level :

1:CLASS2:CLASS3:CLASS4:CLASS5:CLASS6:CLASS7:CLASS9:CLASS11:CLASS